# <Advanced Research Center for Beam Science>Electron Microscopy and Crystal Chemistry

# Advanced Research Center for Beam Science
## – Electron Microscopy and Crystal Chemistry –

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Dr. SCHAPER, Andreas Karl — Philipps University Marburg, Germany, 15 March–13 May

## Scope of Research

Crystallographic and electronic structures of materials and their transformations are studied through direct imaging of atoms or molecules by high-resolution electron spectromicroscopy which realizes energy-filtered imaging and electron energy-loss spectroscopy as well as high resolution imaging. By combining this with scanning probe microscopy, the following subjects are urging: direct structure analysis, electron crystallographic analysis, epitaxial growth of molecules, structure formation in solutions, and fabrication of low-dimensional functional assemblies.


**KEYWORDS**

STEM
ABF
Perovskite Oxide
EELS
Dispersion Curve


### Selected Publications


Minari, T.; Nemoto, T.; Isoda, S., Temperature and Electric-field Dependence of the Mobility of a Single-grain Pentacene Field-effect Transistor, *J. Appl. Phys.*, **99,** 034506 (2006).

Kiyomura, T.; Nemoto, T.; Ogawa, T.; Minari, T.; Yoshida, K.; Kurata, H.; Isoda, S., Thin-Film Phase of Pentacene Film Formed on KCl by Vacuum Deposition, *Jpn. J. Appl. Phys.*, **45,** 401-404 (2006).

Haruta, M.; Kurata, H.; Komatsu, H.; Shimakawa, Y.; Isoda, S., Site-resolved Oxygen K-edge ELNES of Layered Double Perovskite $La_2CuSnO_6$, *Physical Review B*, **80,** 165123 (2009).

Haruta, M.; Kurata, H., Direct Observation of Crystal Defects in an Organic Molecular Crystals of Copper Hexachlorophthalocyanine by STEM-EELS, *Sci. Rep.*, **2,** 252 (2012).

Aso, R.; Kan, D.; Shimakawa, Y.; Kurata, H., Atomic Level Observation of Octahedral Distortions at the Perovskite Oxide Heterointerface, *Sci. Rep.*, **3,** 2214 (2013).

# Topics

## Atomic Level Observation of Octahedral Distortions at the Perovskite Oxide Heterointerface

For perovskite oxides, $ABO_3$, slight octahedral distortions have close links to functional properties. While perovskite oxide heterostructures offer a good platform for controlling functionalities, atomistic understanding of octahedral distortion at the interface has been a challenge as it requires precise measurements of the oxygen atomic positions. Here we demonstrate an approach to clarify distortions at an atomic level using annular bright-field (ABF) imaging in aberration-corrected scanning transmission electron microscopy (STEM), which provides precise mappings of cation and oxygen atomic positions from distortion-minimized images. This technique revealed significant distortions of $RuO_6$ and $ScO_6$ octahedra at the heterointerface between a $SrRuO_3$ (SRO) film and a $GdScO_3$ (GSO) substrate. We also found that structural mismatch was relieved within only four unit cells near the interface by shifting the oxygen atomic positions to accommodate octahedral tilt angle mismatch. The present results underscore the critical role of the oxygen atom in the octahedral connectivity at the perovskite oxide heterointerface.

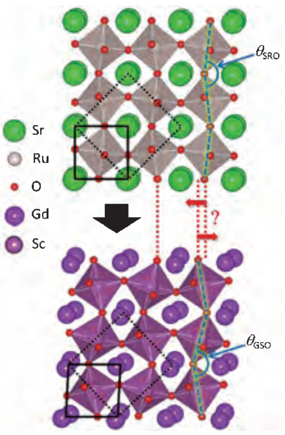


**Figure 1.** Crystal structures of $SrRuO_3$ (SRO) and $GdScO_3$ (GSO).

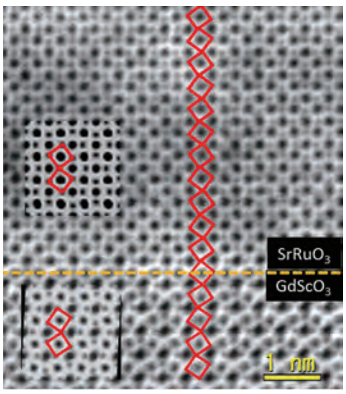


**Figure 2.** Atomic-scale structural characterization of SRO/GSO heterostructure by high-resolution ABF-STEM techniques. The oxygen atoms are clearly visible, revealing the projected shape of each oxygen octahedron and the connectivity of the octahedra across the heterointerface as indicated with the red open squares. Simulated images are also inserted in the image.

## Optical Guided Modes Coupled with Čerenkov Radiation Excited in Si Slab Using Angular-resolved Electron Energy-loss Spectrum

Retardation effects in the valence electron energy-loss spectrum (EELS) of a Si slab are analyzed by angular-resolved EELS. The dispersion curves of the valence spectra excited in a slab are directly observed from a specimen area with several different thicknesses and are interpreted by performing a calculation of the dispersion relation using Kröger's formula. The dispersion curves observed below about 3 eV are attributed to guided modes coupled with Čerenkov radiation (ČR). The coupling between guided modes and ČR is found to be dependent on the sample thickness ($t$). For the sample with $t$>150 nm, the intensity of the guided modes increased linearly with thickness, revealing the coupling with ČR. For $t$<150 nm, however, the intensity of the guided modes rapidly decreased due to a diminished coupling with ČR, resulting from the thickness-dependent dispersion curves of the guided modes.

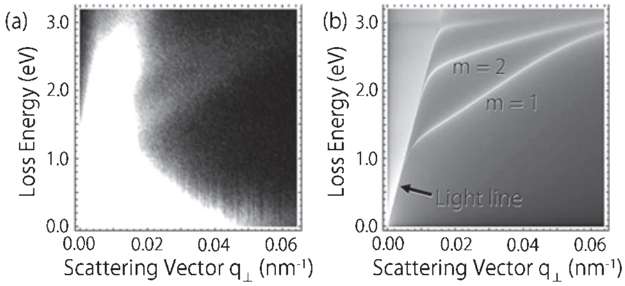


**Figure 3.** Experimental (a) and calculated (b) E-q maps of a Si slab of thickness $t$ = 126 nm. Dispersion curves of 1st & 2nd order guided modes can be seen.